Multiple Gaps and Superfluid Density from Interband Pairing in Iron Oxypnictides

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We study a four-band model for the iron oxypnictides, in which the superconducting properties are assumed to be determined by the interband coupling between hole-like and electron-like Fermi sheets. We show that reasonable parameters can account for the angle-resolved photoemission spectra showing multiple gaps in $Ba_{1-x}K_xFe_2As_2$, and for the temperature dependence of the superfluid density. At the same time, the zero-temperature value of the superfluid density shows a conventional scaling with the number of carriers.

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The discovery of superconductivity in the family of compounds characterized by Fe-As layers[1] is intriguing and challenging. Moreover, at the moment they are the only materials with T_c larger than 40K beside the cuprates. While some properties of these materials are reminiscent of the cuprates (superconductivity induced by doping a magnetic parent compound, layered basic structure), the differences are also remarkable.

Among the peculiarities of the iron oxypnictides not found in cuprates we mention the magnetic nature of Fe and the multi-band character of the band structure. The effect of correlations seems to be weaker than for the cuprates[2], even if also in the latter case the correlation strength may be smaller than usually believed[3]. At the same time, the calculated electron-phonon coupling can not account for the high critical temperatures[4], and some more exotic mechanism is expected to be realized.

The initial efforts in the field focused on $RO_{1-x}F_xFeAs$ and $RO_{1-\delta}FeAs$ (R being a rare earth atom), in which electrons are doped in the parent ROFeAs. Even more recently, a new direction opened thanks to the synthesis of $Ba_{1-x}K_xFe_2As_2$ and $Sr_{1-x}K_xFe_2As_2$, doped by holes. The great advantage of this class of materials is the availability of very large single crystals, which allows for a much more complete and reliable experimental analysis.

Density functional theory (DFT) calculations of the band structure of oxypnictides show that the Fermi surface (FS) is formed by disconnected hole-like pockets centered around the Γ point, and electron-like pockets centered around the M points of the folded Brillouin zone of the FeAs planes. All the pockets essentially arise from the five d-orbitals of Fe, three pockets belonging to the hole-like manifold and two forming the electron-like one[5]. Such a FS topology, along with the magnetic character of the parent compound, motivated one of the first proposal, that assigned to the interband coupling between the two manifold of FS's the role of driving force behind the superconducting phenomenon[5,6]. From a microscopic point of view, the origin of the interband pairing can be associated to spin fluctuations. Indeed, the magnetic ordering vector of the parent compounds roughly connects the two sets of hole and electron FS's, leading to an (approximate) nesting, eventually giving rise to an effective pairing interaction. On the other hand, attractive phonon-induced intraband pairing (or the pairing between FS's of the same nature) is likely to be relatively small.[4] In this perspective, different nesting properties between the various FS sheets can be expected to lead to different strengths of the pairing interaction in the various bands.

Recent angle-resolved photoemission (ARPES) results for undoped[7] and hole-doped $x = 0.4$ $BaFe_2As_2$[8] clearly show that this can indeed be the case. From a broad perspective, ARPES confirms the prediction of DFT about the existence of distinct electron and hole-like pockets. However, only two out of the three hole-like pockets may be resolved around the Γ point, with considerable different areas, and a significant mass renormalization is found in all the bands with respect to DFT.[9] The superconducting (SC) gap opens on all the FS sheets at the same temperature, with a nodeless structure essentially compatible with simple s-wave symmetry. More remarkably, the gap at the smallest hole-like FS and the one at the electron-like sheets are almost identical, while the largest hole-like FS has half of this gap. As we shall see below, this effect is highly non trivial, and requires a proper analysis of the multiband model and of the role of interband interactions. The experimental situation is less clear for the electron-doped materials. A nodeless SC gap at the Γ-FS has been reported for $NdFeAsO_{0.9}F_{0.1}$[10], but no information is available to our knowledge about the gap in the electron-like pocket(s).

Somehow related to the issue of the multiband structure is the behavior of the superfluid density ρ_s, both at zero and finite temperature. The $T = 0$ BCS value of ρ_s is indeed related to the filling and effective masses of the various bands, while its temperature dependence probes via quasiparticle excitations the presence of distinct SC gaps. The aim of this paper is to study a simple model which can capture the main effects of the multiple-gaps opening in $BaFe_2As_2$ superconductors. We will show that a reasonable description of ARPES results and superfluid density can be achieved within a four-band model with

realistic parameters, and that a doping-dependent renormalization of the band structure should be envisaged. Finally, we show that the calculated $T = 0$ value of the superfluid density is in reasonable agreement with the experiments,[11,12,13,14,15] in striking contrast to cuprates, where the anomalous scaling of ρ_s with doping can only be accounted for by including correlation effects[16,17].

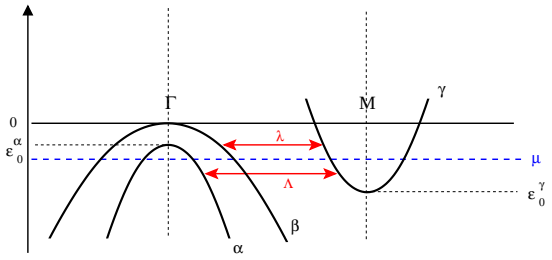

FIG. 1: (Color Online) Schematic of the multiband model used in this work. The two hole bands α, β are centered around the Γ point, the electron bands around the M point.

We consider a four-band model with parabolic dispersion, $\epsilon_i(\mathbf{k}) = \epsilon_0^i \pm t_i(\mathbf{k} - \mathbf{k}_i)^2$, with the plus (minus) sign for the electron (hole) bands and t_i hopping parameter (we will use, unless explicitly stated, units $\hbar = a = 1$, a being the lattice spacing). For the two hole bands around the Γ point, labeled as α and β (according to the notation of Ref. [8]), $\mathbf{k}_i = 0$, while for the two electron bands γ around the M points $\mathbf{k}_i = (\pi, \pi)$. As we mentioned above, the third hole pocket predicted by DFT is not seen around the Γ point, probably because highly degenerate with the α one. Moreover, the two hole pockets are slightly split in the undoped system.[7] Thus, we choose the reference energy such that $\epsilon_0^\beta = 0$, while ϵ_0^α and ϵ_0^γ are in general different from zero, see Fig. 1. For simplicity, we assume that the two electron bands are equal and isotropic around the M points, even though both DFT and experiments show that they are slightly elongated along the k_x and k_y directions. Within a BCS-like approach, the pairing Hamiltonian can be written as:

$$H = \sum_{i,\mathbf{k}\sigma} \epsilon_i(\mathbf{k}) c^+_{i,\mathbf{k}\sigma} c_{i,\mathbf{k}\sigma} + \sum_{\substack{i\neq j \\ \mathbf{k},\mathbf{k}'}} V_{i,j} c^+_{i,\mathbf{k}\uparrow} c^+_{i,-\mathbf{k}\downarrow} c_{j,-\mathbf{k}'\downarrow} c_{j,\mathbf{k}'\uparrow}, \quad (1)$$

where $c^+_{i,\mathbf{k}}$ creates an electron in the i-th band ($i = \alpha, \beta, \gamma$), and as we discussed above we neglect intraband pairing. Moreover, the similar size of the FS for the α and γ bands suggests that the largest pairing acts between these two FS sheets, which are strongly nested, while the β and γ bands are less coupled. These conditions are implemented in (1) by taking $V_{\alpha\beta} = 0$, $V_{\beta\gamma} = \lambda$ and $V_{\alpha\gamma} = \Lambda > \lambda$. As it has been noticed in Ref.[5,6], for inter-band mechanisms it is not necessary that the interaction is attractive (at least at low energy), as it happens for intra-band mechanisms. However, if $\Lambda, \lambda > 0$ one sees that the order parameters must have different sign on different kind of FS sheets, i.e. $\mathrm{sign}\Delta_{\alpha,\beta} = -\mathrm{sign}\Delta_\gamma$. The resulting set of self-consistent equations for the absolute values of the gaps is a straightforward extension of the usual BCS equations:

$$\Delta_\alpha = \Lambda \Delta_\gamma 2\Pi_\gamma \quad (2)$$
$$\Delta_\beta = \lambda \Delta_\gamma 2\Pi_\gamma \quad (3)$$
$$\Delta_\gamma = \Lambda \Delta_\alpha \Pi_\alpha + \lambda \Delta_\beta \Pi_\beta \quad (4)$$

where Δ_i is the gap in the i-th band, whose dispersion is now $E_{i,\mathbf{k}} = \sqrt{\xi_i^2(\mathbf{k}) + \Delta_i^2}$, with $\xi_i \equiv \epsilon_i - \mu$. The Π_i are the particle-particle bubbles, given by $\Pi_i = N_i \int_0^{\omega_0} d\xi (1/E_i) \tanh(E_i/2T)$, where the pairing is only effective for states in a range $|\xi| < \omega_0$ around the Fermi level and $N_i = 1/4\pi t_i$ is the density of states (DOS) of each band. Here we use $\omega_0 = 20$ meV, i.e. of the order of the smallest Fermi energy in the different sheets. Along with Eqs. (2)-(4) we must solve self-consistently the equation for the particle number $n = n_\alpha + n_\beta + 2n_\gamma$, where $n = 4$ is the half filling. At the present stage the agreement between the experimental dispersion and the DFT bandstructure is hardly satisfactory[9], therefore we extract the band parameters from the experimental data of Ref.[7] for undoped $BaFe_2As_2$. Here one has $t_\alpha = 90$ meV, $t_\beta = 39$ meV and $t_\gamma = 45$ meV, with a band splitting $\epsilon_0^\alpha = -10$ meV and $\epsilon_0^\gamma = -45$ meV. However, in a rigid-band picture, with these parameters at the doping $x = 0.4$ the electron pockets would be empty. Moreover, as we shall see below in Fig. 2b, with these parameters the gap values in the α and γ bands would be quite different, in contrast to what measured in Ref.[8]. We thus proceed by assuming a band renormalization with respect to half-filling to obtain $\Delta_\alpha \simeq \Delta_\gamma$, and $\Delta_\alpha = 2\Delta_\beta$ from Eqs. (2)-(4), where the gap values depend only on the DOS and on the coupling. The latter condition is always realized for $\lambda = \Lambda/2$. The former condition instead can be obtained with slightly renormalized bands, i.e. we use $t_\alpha = 65$ meV, $t_\beta = 25$ meV and $t_\gamma = 60$ meV. Notice that if a third hole pocket of the same size of the α one is present, even if not explicitly observed by ARPES, this would just require to slightly change the parameters to compensate the substitution of $\Pi_\alpha \to 2\Pi_\alpha$ in Eq. (4).

Once the DOS are fixed by the gap values, we tune the band splitting according to the FS areas A_i measured in Ref.[8]. In particular, it is observed that $A_\alpha/A_\beta = 2/9$. Notice that if α and β bands were degenerate (or nearly degenerate) at the Γ point this A_α/A_β ratio would require a very large anisotropy between the hole bands, $t_\beta = t_\alpha(2/9)$, which in turn would not allow the condition $\Delta_\alpha \simeq \Delta_\gamma$ to be fulfilled. Thus, to justify the ratios of the FS areas we should assume a splitting of the hole bands at the Γ point, even larger than what measured at half-filling[7]. This enhancement of the splitting can be associated to a different Hartree shift of the two bands, arising from a particle-hole decoupling of the interband interaction. Imposing the FS ratios suggested in Ref.[8] we determine $\epsilon_0^\gamma = -71$ meV and $\epsilon_0^\alpha = -25$ meV (so that $\mu \simeq -60$ meV). In Fig. 2a we show the results for the gaps using $\Lambda = 260$ meV, which at low T are in good agreement with the experimental results of Ref.[8], even if

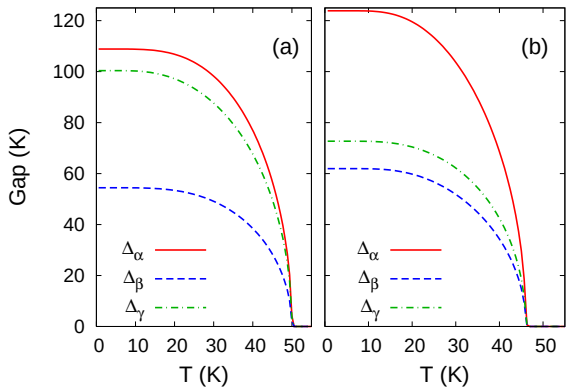

FIG. 2: (Color Online) (a): Temperature dependence of the SC gaps in the hole and electron bands. The parameter values are optimized to obtain the same gap value in the α and γ bands (values in eV). Moreover, we used $\lambda = \Lambda/2$ to have $\Delta_\beta = \Delta_\alpha/2$. (b): SC gaps for the hopping parameters estimated from ARPES measurements of Ref.[7] at half-filling.

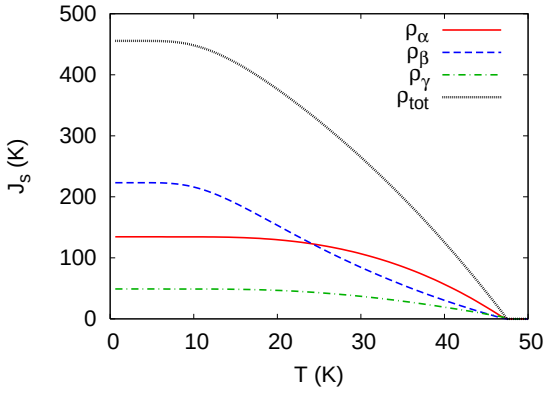

FIG. 3: (Color Online) Temperature dependence of the superfluid density in units of Eq. (6) for the various bands.

a larger T_c is found here because fluctuation effects, that are expected to be important in 2D, are not included. We point out that in a multiband system dominated by off-diagonal (interband) coupling, deviations from the BCS value of $2\Delta/T_c$ in each band can be obtained without invoking exotic mechanisms. In Fig. 2a we find $2\Delta_\beta/T_c = 2$ and $2\Delta_\alpha/T_c = 4$, and further enhancement could be expected after the inclusion of fluctuation effects.

When multiple gaps are present, one may expect a signature on the temperature behavior of the superfluid density ρ_s. For a generic lattice dispersion $\epsilon_{\mathbf{k}}$, the superfluid density at BCS level is given by:

$$\rho_s = \int \frac{d^2\mathbf{k}}{2\pi} \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_\alpha^2} \left(1 - \frac{\epsilon_{\mathbf{k}} - \mu}{E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2T}\right)\right) + + 2 \int \frac{d^2\mathbf{k}}{2\pi} \left(\frac{\partial \epsilon_{\mathbf{k}}}{\partial k_\alpha}\right)^2 \frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}, \quad (5)$$

where $f(x) = [1 + \exp(x/T)]^{-1}$ is the Fermi function. Let us first consider the electron bands γ: since they are almost empty, we can approximate the full dispersion $\epsilon_{\mathbf{k}}$ with the parabolic band ϵ_γ introduced above, so that the previous equation reduces to $\rho_s^\gamma = 2t_\gamma n_\gamma + 4t_\gamma N_\gamma \int d\epsilon\, \epsilon f'(E_\gamma)$. As $T \to 0$ the quasiparticle excitations vanish, due to the derivative $f'(E_\gamma)$, and the usual result $\rho_s^\gamma = 2t_\gamma n_\gamma$ is recovered. For hole bands, a similar expression can be used after a particle-hole transformation, which insures that only the hole states at the top of the band contribute to the superfluid density, i.e. $\rho_s^\alpha = 2t_\alpha(2 - n_\alpha)$ at $T = 0$.

The results for the temperature dependence of the superfluid density for the same parameters of Fig. 2a are shown in Fig. 3, where we plot the total ρ_s together with the contributions from the single bands. In the β band, which has the smallest gap, the clear signature of the two different order parameters can be seen most clearly, while the two other bands have a more standard behavior. As we observed above, for the β-band $2\Delta_\beta/T_c = 2$, i.e. it is smaller than the BCS value. This means that $\Delta(T)$ is finite and sizable in a regime of temperature where it would be zero if not coupled to another band. As a consequence, at low T ρ_s^β decreases quite rapidly, as it would vanish at a temperature proportional to Δ_β, while at higher temperature the depletion softens in a tail which closes at the higher T_c determined by the interband coupling. The possibility to observe a clear change of curvature in the total superfluid response ρ_s^{tot} depends on the relative filling of the band with the smaller gap. In Fig. 3 we show that the presence of the multiple gaps leads to deviations of $\rho_s^{tot}(T)$ with respect to the single-band case, but with no upward curvature as in $\rho_s^\beta(T)$. We notice that ρ_s^{tot} strongly resembles the one reported recently in Ref.[11] in a $Ba_{0.55}K_{0.45}Fe_2As_2$ compound with similar doping of the one studied by ARPES in Ref.[8].

More intriguing is instead the temperature dependence observed in several electron-doped $LaO_{1-x}F_xFeAs$[12,13] and $NdO_{1-x}F_xFeAs$[14] compounds, where the measured ρ_s resembles the one we find for the β band. This effect is particularly pronounced in $LaO_{1-x}F_xFeAs$ for $x > 0.1$, and suggests that the smaller gap is formed on the electron part of the FS, which is expected to give the larger contribution to the superfluid response in electron-doped compounds. Even though some indications of multiple gaps in $LaO_{1-x}F_xFeAs$[18] already exist, a clear experimental observation of the gap opening on the different FS sheets is still lacking.

We finally comment on the $T = 0$ value of the superfluid density, which is proportional to the Fermi energy within our BCS scheme, and it is therefore of the order of several hundreds of K. This energy scale is comparable to the values currently available from penetration-depth measurements in both hole-doped[11,15] and electron-doped[12,13,14] oxypnictides. To make a direct comparison with the experiments, we recall that in two dimensions the quantity $J_s = \hbar^2 n_s^{2d}/m$ is an energy, where n_s^{2d} is a two-dimensional density of superfluid carriers. By considering each plane as the basic 2D unit,

one can relate n_s^{2d} and J_s to the measured penetration depth λ as:

$$J_s = \frac{\hbar^2 n_s^{2d}}{m} = \frac{\hbar^2 c^2}{4\pi e^2}\frac{d}{\lambda^2} = 2.48\frac{d[\mathring{A}]}{\lambda^2[(\mu m)^2]}K \qquad (6)$$

where d is the interlayer spacing, which ranges between 4.3-6.6 Å in oxypnictides. The penetration depth of a $Ba_{0.6}K_{0.4}Fe_2As_2$ sample has been estimated in Ref.[15] from infrared measurements as $\lambda = 0.208$ μm. This gives according to Eq. (6) $J_s \simeq 380$ K, which is not much lower that the value we estimated above assuming the clean limit. Moreover, since the optical-conductivity measurements of Ref.[15] suggest that the sample is in the dirty limit, we would expect that only a fraction of the ρ_s estimated from the (renormalized) band structure will actually condense in the SC phase. We can then conclude that the measured superfluid-density values are quite consistent with band-structure calculations. For this reason, the observed similarity of the relation of $1/\lambda^2$ vs T_c in oxypnictides and cuprates superconductors[12] should *not* be taken as a signature of similar unconventional behavior in the two classes of materials. Indeed, in cuprate superconductors the number of carriers is large, because one is doping the system with respect to half-filling, where the superfluid density is expected to attain its maximum value in a hypothetical uncorrelated system. In other words, one would expect $\rho_s \sim (1-x)t$, while one measures values of order $\rho_s \sim xt$, where x is the doping and t the typical hopping parameter. For this reason, correlation effects as the proximity to a Mott insulator[16] or enhanced phase fluctuations[17] have been invoked as possible explanation of the low superfluid density in cuprates. Instead, in oxypnictides the system has a low superfluid density because an almost full hole band has a vanishing contribution to ρ_s, and one expects $\rho_s \sim xt$ which is indeed near to the experimental values.

In conclusion, we have presented calculations in a four-band model built on the basis of the experimental results on $BaFe_2As_2$, assuming that the pairing arises from the interaction between hole-like and electron-like Fermi surfaces, with different strengths due to different nesting properties of the various FS sheets. Within our multi-band BCS approach we determine parameters that account for the multiple gaps recently observed by Ding *et al.*[8]. Using the same parameters, we compute the superfluid density, which does not show striking signatures of the multiple gaps, in agreement with experiments. The same agreement holds for its zero-temperature value, which scales with the small density of carriers. This has to be contrasted to the case of cuprates, where the smallness of ρ_s is associated to correlation effects.

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[1] Y. Kamihara *et al.*, J. Am Chem. Soc. **128**, 10012 (2006); *ibid.* **130**, 3296 (2008)

[2] K. Haule, J. H. Shim, and G. Kotliar, Phys. Rev. Lett. **100**, 226402 (2008)

[3] A. Comanac, L. de' Medici, M. Capone, and A. J. Millis, Nat. Phys. **4**, 287 (2008)

[4] L. Boeri, O. V. Dolgov, and A. A. Golubev, Phys. Rev. Lett. **101**, 026403 (2008)

[5] I. I. Mazin, D. J. Singh, M. D. Johannes, M. H. Du, arXiv:0803.2740 ; I. I. Mazin, L. Boeri, K. Kopernik, D. J. Singh, arXiv:0806.1869

[6] F. Wang, H. Zhai, Y. Ran, A. Vishwanath, and D. -H. Lee, arXiv:0805:3343; M. M. Korshunov and I. Eremin, arXiv:0803:3325; A.V. Chubukov, D. Efremov, I. Eremin, arXiv:0807.3735

[7] L.X.Yang, Y. Zhang, H. W. Ou, J. F. Zhao, D. W. Shen, B. Zhou, J. Wei, F. Chen, M. Xu, C. He, Y. Chen, Z. D. Wang, X. F. Wang, T. Wu, G. Wu, X. H. Chen, M. Arita, K. Shimada, M. Taniguchi, Z. Y. Lu, T. Xiang, D. L. Feng, arXiv:0806.2627

[8] H. Ding, P. Richard, K. Nakayama, K. Sugawara, T. Arakane, Y. Sekiba, A. Takayama, S. Souma, T. Sato, T. Takahashi, Z. Wang, X. Dai, Z. Fang, G. F. Chen, J. L. Luo and N. L. Wang, Europhys. Lett. **83**, 47001 (2008)

[9] I.A. Nekrasov, Z.V. Pchelkina, M.V. Sadovskii, arXiv:0806.2630; D.J. Singh, arXiv:080.2643

[10] C. Liu, T. Kondo, M. E. Tillman, R. Gordon, G. D. Samolyuk, Y. Lee, C. Martin, J. L. McChesney, S. Bud'ko, M. A. Tanatar, E. Rotenberg, P. C. Canfield, R. Prozorov, B. N. Harmon, A. Kaminski, arXiv:0806.3453; T. Kondo, A. F. Santander-Syro, O. Copie, C. Liu, M. E. Tillman, E. D. Mun, J. Schmalian, S. L. Bud'ko, M. A. Tanatar, P. C. Canfield, A. Kaminski, arXiv:0807.0815

[11] A. A. Aczel, E. Baggio-Saitovitch, S. L. Budko, P. C. Canfield, J. P. Carlo, G. F. Chen, P. Dai, T. Goko, W. Z. Hu, G. M. Luke, J. L. Luo, N. Ni, D. R. Sanchez-Candela, F. F. Tafti, N. L. Wang, T. J. Williams, W. Yu, Y. J. Uemura, arXiv:0807.1044

[12] H. Luetkens, H.-H. Klauss, R. Khasanov, A. Amato, R. Klingeler, I. Hellmann, N. Leps, A. Kondrat, C.Hess, A. Köhler, G. Behr, J. Werner, B. Büchner, arXiv:0804.3111.

[13] H. Luetkens, H.-H. Klauss, M. Kraken, F. J. Litterst, T. Dellmann, R. Klingeler, C. Hess, R. Khasanov, A. Amato, C. Baines, J. Hamann-Borrero, N. Leps, A. Kondrat, G. Behr, J. Werner, B. Buechner, arXiv:0806.3533.

[14] C. Martin, R. T. Gordon, M. A. Tanatar, M. D. Vannette, M. E. Tillman, E. D. Mun, P. C. Canfield, V. G. Kogan, G. D. Samolyuk, J. Schmalian, R. Prozorov, arXiv:0807.0876

[15] G. Li, W. Z. Hu, J. Dong, Z. Li, P. Zheng, G. F. Chen, J. L. Luo, N. L. Wang, arXiv:0807.1094

[16] M. Capone, M. Fabrizio, C. Castellani, E. Tosatti, Phys. Rev. Lett. **93**, 047001 (2004)

[17] See L. Benfatto, A. Toschi, and S. Caprara, Phys. Rev. B. 69, 184510 (2004) and references therein.

[18] R. S. Gonnelli, D. Daghero, M. Tortello, G. A. Ummarino, V. A. Stepanov, J. S. Kim, R. K. Kremer, arXiv:0807.3149